Spin Transport in the XXZ Chain at Finite Temperature and Momentum

Robin Steinigeweg[1,*] and Wolfram Brenig[1]

[1]*Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany*

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We investigate the role of momentum for the transport of magnetization in the spin-1/2 Heisenberg chain above the isotropic point at finite temperature and momentum. Using numerical and analytical approaches, we analyze the autocorrelations of density and current and observe a finite region of the Brillouin zone with diffusive dynamics below a cut-off momentum, and a diffusion constant independent of momentum and time, which scales inversely with anisotropy. Lowering the temperature over a wide range, starting from infinity, the diffusion constant is found to increase strongly while the cut-off momentum for diffusion decreases. Above the cut-off momentum diffusion breaks down completely.

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Understanding spin transport in quantum many-particle systems is a fundamental challenge to physics, of immediate relevance to future information technologies [1], and intimately related to timely issues of dynamics and thermalization in a more broader context [2]. While conventional spin conductors like silicon [3], III-V semiconductors [4], carbon nanotubes [5], or graphene [6] necessarily feature spins which are associated with itinerant charge carriers, insulating quantum magnets may open new perspectives for spin transport, with pure magnetization currents flowing solely by virtue of exchange interactions. Magnetic transport in one-dimensional (1D) quantum magnets has experienced an upsurge of interest in the last decade due to the discovery of very large magnetic *heat* conduction [7] with mean free paths above $1\mu m$ [8]. Genuine *spin* transport in quantum magnets remains yet to be observed experimentally, however long nuclear magnetic relaxation times [9] have been established, which even allow for manipulation with magnetic fields [10].

Theoretically, significant attention has been devoted to spin transport in 1D quantum magnets, see Refs. 11 and 12 for reviews. The dissipation of spin currents is a key issue in this context and has been analyzed extensively at zero momentum and frequency in connection with the spin Drude weight [13]. Spin current dynamics at *finite* momentum remains one of the open questions. In this Letter, we will address this question for the antiferromagnetic and anisotropic spin-1/2 Heisenberg (XXZ) chain

$$H = J \sum_{r}^{N} (S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta\, S_r^z S_{r+1}^z)\,, \qquad (1)$$

where S_r^i $(i = x, y, z)$ are the components of spin-1/2 operators at site r, N denotes the number of sites, $J > 0$ represents the exchange coupling constant, and Δ is the anisotropy. The XXZ chain is a fundamental model to describe magnetic properties of interacting electrons. It is relevant to the physics of low-dimensional quantum magnets [14], ultra-cold atoms [15], nanostructures [16], and – seemingly unrelated – fields such as string theory [17] and quantum Hall systems [18].

Early analysis of the time-dependent correlation function of the local spin density has been performed in the high-temperature limit, $T = \infty$, suggesting the absence of spin diffusion for $0 \leqslant \Delta \leqslant 1$ [19]. Subsequent, studies have concentrated on the spin Drude weight at zero momentum $q = 0$ [13], allowing for no conclusions on diffusion laws at finite momentum. First low-temperature quantum Monte-Carlo studies at $q \neq 0$ [20] found no evidence for spin diffusion; however, more recent results from bosonization and transfer-matrix renormalization group [21] as well as quantum Monte-Carlo [22] are consistent with finite-frequency spin diffusion in the small-momentum regime, at $\Delta = 1$ and for low temperatures $T \ll J$, with a spin diffusion constant D which diverges $\propto 1/T \ln T$. The physics at intermediate temperatures and arbitrary momenta remains undisclosed.

Therefore, in this Letter, we consider the transport of magnetization by analyzing autocorrelations of spin density and current at finite momenta, covering the complete Brillouin zone, and at intermediate temperatures $0.5J \leqslant T \leqslant \infty$ $(\hbar = k_B = 1)$. We focus on the case of finite anisotropy $\Delta > 1$, where Eq. (1) features a gapped ground state. Using a combination of exact diagonalization and perturbation theory, we uncover a regime of diffusive transport below a finite critical momentum q_D. In this regime, density modes at fixed momentum q decay with a diffusion constant D_q and our analysis is consistent with D_q *independent* of momentum and inversely proportional to the anisotropy. As the temperature is lowered from $T = \infty$, we observe a decrease of the critical momentum and an almost exponential increase of the diffusion constant. We provide evidence for a complete breakdown of diffusion above the critical momentum.

We begin by introducing the generalized diffusion coefficient as a quantity suitable to describe the evolution of a harmonic spin density profile close to equilibrium, i.e., in the linear response regime. To this end, the central quantities we analyze are the autocorrela-

tion functions $C_{S,q}(t) = \mathrm{Re}\langle S^z_q(t) S^z_{-q}\rangle/N$ and $C_{J,q}(t) = \mathrm{Re}\langle J^z_q(t) J^z_{-q}\rangle/N$ of the spin density $S^z_q = \sum_r e^{\imath qr} S^z_r$ and the spin current $J^z_q = J\sum_r e^{\imath qr}(S^x_r S^y_{r+1} - S^y_r S^x_{r+1})$ at momentum $q = 2\pi k/N$ [23], where Re indicates the real part, $\langle \ldots \rangle$ denotes the canonical equilibrium average at the inverse temperature $\beta = 1/T$, and t represents the time. Since the density S^z_q and the current J^z_q are connected by the lattice continuity equation $\partial_t S^z_q = (1 - e^{\imath q}) J^z_q$, the autocorrelations are related by $\partial^2_t C_{S,q}(t) = -\tilde{q}^2 C_{J,q}(t)$ with the abbreviation $\tilde{q}^2 = 2(1-\cos q)$. The generalized, time- and momentum-dependent diffusion coefficient is *defined* via

$$D_q(t) = \frac{\partial_t C_{S,q}(t)}{-\tilde{q}^2 C_{S,q}(t)} = \frac{I^1_q(t)}{C_{S,q}(0) - \tilde{q}^2 I^2_q(t)} \, . \qquad (2)$$

To arrive at the right-hand expression in Eq. (2), we integrate the continuity equation twice, using $\partial_t C_{S,q}(t)|_{t=0} = 0$ and introducing the two integrals $I^1_q(t) = \int_0^t \mathrm{d}t' \, C_{J,q}(t')$ and $I^2_q(t) = \int_0^t \mathrm{d}t' \, I^1_q(t')$.

The left-hand expression in Eq. (2) identifies the quantity $\tilde{q}^2 D_q(t)$ with the instantaneous decay rate, at time t, of a spin density profile with wave vector q close to equilibrium. Fick's law corresponds to the case of $D_q(t) = \text{const}$. The main goal of this Letter is to analyze the time- and momentum-dependence of this quantity versus temperature. We emphasize that a complete knowledge of this dependence allows to propagate arbitrarily shaped spin density profiles in time. This does not only share a common interest with time-dependent density-matrix renormalization group studies [24], yet confined to zero temperature, but even more so may be of relevance to laser pulse induced time-dependent transport measurements, including recently proposed time-of-flight and thermal imaging techniques [25].

Qualitatively, the variation of $D_q(t)$ versus t can be understood from a standard relaxation-time approximation, in which the current autocorrelation $C_{J,q}(t) = \exp(-t/t_q)\, C_{J,q}(0)$ decays exponentially. For short times, $t \ll t_q$, Eq. (2) then yields $D_q(t) \sim 1 - e^{-t/t_q}$, which starts with a linear increase, $D_q(t) \propto t$, and turns into a 'plateau' $D_q(t) \approx$ const., starting at $t = \tau_q \gtrsim t_q$. This plateau marks the hydrodynamic regime. Namely, proceeding to the long-time limit, i.e. for $t \gg t_q$, and to the long-wavelength limit, i.e. for $\tilde{q}^2(t - t_q) D_q \ll 1$, Eq. (2) leads to a time-*independent* diffusion constant $D_q(t) = D_0 + \mathcal{O}(\tilde{q}^2)$, where $D_q = t_q \, C_{J,q}(0)/C_{S,q}(0)$, which is equivalent to Einstein's relation [26], and $D_0 = D_{q=0}$. In principle, partial conservation of currents at $q = 0$, i.e. the impact of a finite Drude weight at zero frequency [13], can also be included into this qualitative picture. For that case the exponential decay of $C_{J,0}(t)$ has to be leveled off into $C_{J,0}(t \to \infty) = \text{const.} > 0$. This leads to a linear increase $D_0(t \to \infty) \propto t$. However, the Drude weight will not be an issue in this Letter. In fact, there is no zero-frequency contribution of currents at $q \neq 0$, which follows directly from the continuity equation.

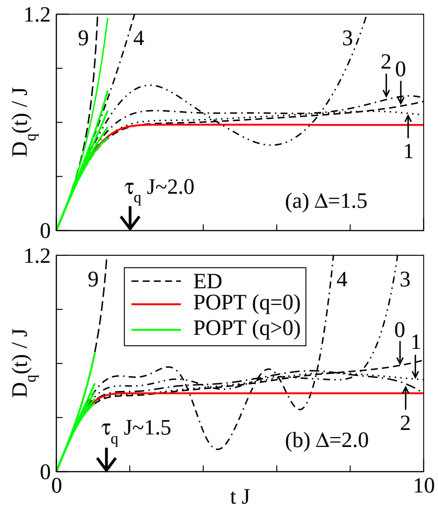

FIG. 1. (color online) The time- and momentum-dependent diffusion coefficient $D_q(t)$ at $\beta = 0$ and (a) $\Delta = 1.5$, (b) $\Delta = 2.0$. ED results are shown for $N = 18$ and $q/(2\pi/N) = 0, 1, 2, 3, 4$, and 9 (non-solid curves). POPT results are shown for $q = 0$ (red/dark-colored, solid curves) and $q > 0$ (green/light-colored, solid curves). Thick arrows on the tJ-axis mark the locations of the current decay time τ_q.

While the gross feature of the preceding relaxation-time *ansatz* can serve as a guideline to interpret the results of unbiased exact diagonalization data, on which we will report later, it is not justified *a priori*. Therefore, and to gain a deeper insight into the high-temperature current dynamics generated by the Heisenberg model, we will first turn to a quantitative discussion using an analytical method. This method employs the projection operator perturbation theory (POPT) of Ref. 27, which allows to derive a rate equation $\partial_t C_{J[S],q}(t) = -\gamma_{J[S],q}(t)\, C_{J[S],q}(t)$ for the current [density] autocorrelation. This rate equation gives access to $D_q(t)$ through the right-hand [central] expression in Eq. (2). The POPT yields a short-time expansion for the decay rate $\gamma_{J[S],q}(t)$, the terms of which can be evaluated from a decomposition $H = H_0 + H_1$, if the observable of the autocorrelation $C_{J[S],q}(t)$ is a conserved quantity for the unperturbed Hamiltonian H_0. For the current, we choose the XY model for H_0, in which J_q is conserved *only* at $q = 0$. For the density, we choose the Ising model for H_0, in which S_q is conserved for *all* q. Then for short times we obtain approximately:

$$\frac{\gamma_{J,0}(t)}{\Delta J} \approx \frac{\Delta J t}{2} + \frac{(\Delta J t)^3}{24} + \mathcal{O}[(\Delta J t)^5], \; tJ \lesssim 1.5 \qquad (3)$$

$$\frac{\gamma_{S,q}(t)}{\tilde{q} J} \approx \frac{\tilde{q} J t}{2} + \frac{(\tilde{q} J t)^3}{16} + \mathcal{O}[(\tilde{q} J t)^5], \; tJ \lesssim \frac{2.1}{\Delta} \qquad (4)$$

For the full quantitative evaluation of $D_q(t)$ we determine the leading-order term in Eqs. (3) and (4) numerically exact, following the scheme in Ref. 27, which leads to small changes only. We note that for a complete integration of

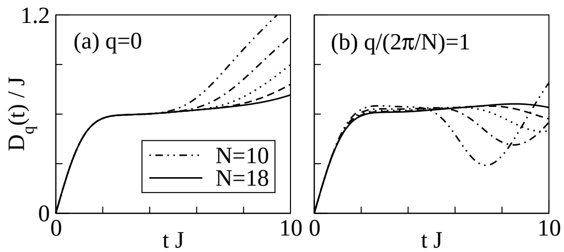

FIG. 2. (color online) Finite-size scaling results for the diffusion coefficient $D_q(t)$ at (a) $q = 0$, (b) $q/(2\pi/N) = 1$ for different $N = 10, 12, \ldots, 18$ at $\beta = 0$ and $\Delta = 1.5$. In (a) finite-size variations can be neglected for $tJ \lesssim 10$ at $N = 18$. While $q =$ const. cannot be maintained in (b), the tendency is similar to (a).

Eq. (2) the high-temperature limits of the static correlation functions are needed, i.e. $C_{J[S],q}(0) = 1/8$ [1/4].

For $q = 0$, we obtain from the POPT and the right-hand expression in Eq. (2) a leading order prediction as follows: the current autocorrelation $C_{J,0}(t)$ decays even *stronger* than in a simple relaxation-time approximation, i.e. according to a Gaussian, and the diffusion coefficient $D_0(t)$ is an error function. This prediction is consistent with using Eq. (3) for *all* times, which is justified because the current relaxation time from Eq. (3) is $t_0 J \approx 1.9/\Delta$, $C_{J,0}(t_0)/C_{J,0}(0) = 1/e$. Therefore for $\Delta = 1.5$ or 2.0, as in this Letter, $D_0(t)$ has saturated for times within $tJ \lesssim 1.5$. The resulting quantitative $D_0(t)$ is shown in Fig. 1 (red/dark-colored, solid curves): Here, $D_0(t)$ first increases linearly but then saturates at a constant value $D_0 J \approx 0.88/\Delta$, which is reached at $tJ \gtrsim \tau_0 J \approx 3.0/\Delta$. For the remainder of this Letter we refer to the saturation time τ_q as the 'current relaxation time', rather than t_q, since it can be extracted more precisely from later numerical data. We emphasize that our value of D_0 agrees remarkably well with other approaches in Refs. 28 and 29. It is worth to mention that, for $\Delta \to \infty$, the $1/\Delta$-scaling of D_0 may break down due to possible recurrences of $C_{J,0}(t)$, see also Ref. 32 for an alternative point of view.

For $q \neq 0$, we obtain from the POPT and the central expression in Eq. (2) a prediction for the full momentum-dependence of $D_q(t)$. This prediction is only valid at short times, set by Eq. (4). The resulting quantitative $D_q(t)$ is depicted in Fig. 1 (green/light-colored, solid curves). Clearly, $D_q(t)$ is *not* constant in the short-time domain as a function of q. The q-dependence arises from the next-to-leading order term of the POPT and becomes significant for momenta above $q \sim 0.2\pi\,\Delta$, at $\Delta = 1.5$ and 2.0, and is particularly evident for $q = \pi$.

In order to complete the picture at $\beta = 0$ for arbitrary momenta and times we apply exact diagonalization (ED) to chains of length $N = 18$, allowing for a q-grid with $\delta q \approx 0.11\pi$. Figure 1 depicts our results for $D_q(t)$. Several comments are in order. First, Figs. 1 (a) and (b) show a convincing agreement between ED and both POPTs within their respective ranges of validity, which corroborates our analysis. Next, a given density mode at wave vector q shows the signature of a diffusive decay if there is a plateau with $D_q(t) \approx$ const. within a 'long-time' window $\tau_q \lesssim t \lesssim t_D$ with $\tau_q \ll t_D$. Clearly, Fig. 1 shows that the first three (four) momenta for $\Delta = 1.5$ (2.0) feature such plateaus. Long-time deviations from this behavior can have several origins, such as finite-size effects, finite Drude weights, or other low-frequency anomalies. Most remarkable, the plateau values of $D_q(\tau_q \lesssim t \lesssim t_D) \approx D_0$ and $\tau_q \approx \tau_0$ are *independent* of momentum, to within the typical finite-size variations which occur for $N = 16 \to 18$. Finite-size effects are further quantified in Fig. 2 for the interval $tJ \lesssim 10$. While a constant finite q cannot be maintained as N varies, it is still obvious that system sizes of $N = 18$ are completely sufficient to determine D_q at the plateau. The weak dependence on q has to be contrasted against the significant q-dependence for larger momenta. In agreement with the POPT for $q = 0$, the values of D_0 and τ_0 from ED can be scaled onto a single expression for the two anisotropies studied, namely, $D_0\,J \approx 0.88/\Delta$ for $t\,J \gtrsim \tau_0\,J \approx 3.0/\Delta$. This is one of the main results of this Letter, i.e., the existence of an extended momentum-space region with a q-independent diffusion constant $\propto 1/\Delta$. Clearly, the number of momenta to which the diffusion criterion applies is smaller in Fig. 1 (a) than in (b). For both $\Delta = 1.5$ and 2.0, we find no indications of diffusion for $q \gtrsim 0.22\pi\Delta \equiv q_D$. Instead, $D_{q>q_D}(t)$ displays divergent behavior due to oscillations of $C_{S,q}(t)$ with time, preventing diffusive behavior to occur. These oscillations have already been reported in Ref. 30 for smaller Δ.

We emphasize that ED results for the *spectra* $C_{J[S],q}(\omega)$ at small q versus frequency ω agree with our interpretation from the time domain. E.g., focusing on $\Delta = 1.5$, Fig. 3 (a) shows that the spectrum $C_{J,q}(\omega)/C_{S,q}(t=0)$ is consistent with a Gaussian of height $D_0 J \approx 0.59$, as predicted by the POPT at $q = 0$. The low-frequency behavior is still governed by finite-size effects and deviations from the Gaussian occur at a frequency scale

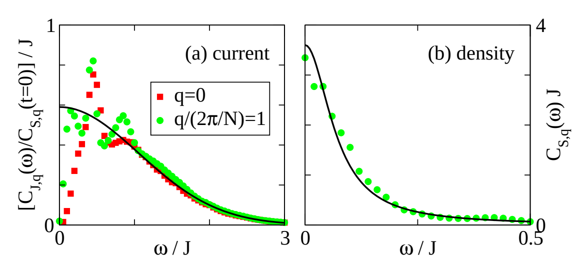

FIG. 3. (color online) Spectrum of the (a) current and (b) density autocorrelation at $\beta = 0$ and $\Delta = 1.5$. ED results are shown for $N = 18$ (symbols). In (a) a Gaussian with height D_0 and in (b) a Lorentzian with width $\tilde{q}^2\,D_0$ are indicated for comparison (curves), using $D_0 J \approx 0.59$ from the POPT.

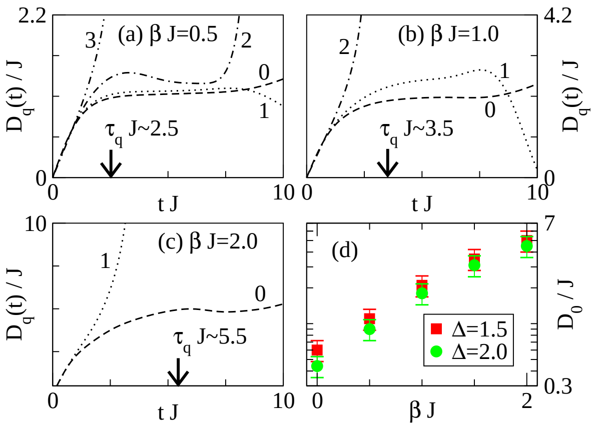

FIG. 4. (color online) (a)–(c) ED results for the diffusion coefficient $D_q(t)$ at different $\beta > 0$ for $\Delta = 1.5$ and $N = 18$ (curves). Thick arrows mark the approximate locations of the current decay time τ_q. (d) The resulting diffusion constant D_0 versus β for $\Delta = 1.5$ (squares) and $\Delta = 2.0$ (circles), which can be determined with a precision of 20% (error bars).

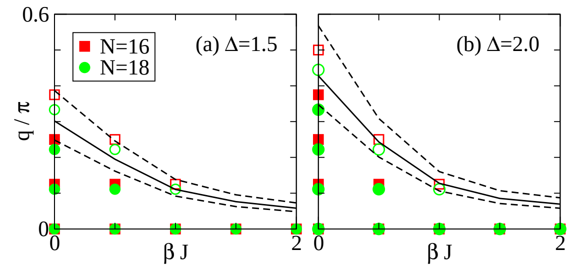

FIG. 5. (color online) The diffusive range of momenta q versus β for (a) $\Delta = 1.5$ and (b) $\Delta = 2.0$. ED results are shown for $N = 16$ (squares) and $N = 18$ (circles). [Open symbols are borderline values, see Fig. 1 and Fig. 4 (a)–(c).] The curve $\tilde{q}^2 D_0 \tau_0 = 1$ is indicated for comparison (solid curves). (Dashed curves estimate errors for D_0 and τ_0.)

$\omega/J \lesssim 1$, which is independent of q. This agrees with the q-independent time scale in Fig. 2, where finite-size effects set in. Similar spectra of $C_{J,q}(\omega)$ have been obtained in Ref. 31 for $q = 0$. Note that the (finite size) $q = 0$ Drude weight at $\omega = 0$ is not shown in Fig. 3 (a). Figure 3 (b) shows that $C_{S,q}(\omega)$ is consistent with a Lorentzian of width $\tilde{q}^2 D_0$, again $D_0 J \approx 0.59$, as expected for diffusive density decay.

Now we turn to the effects of temperature by increasing β from 0 to $\beta J = 2$. Since the POPT is not applicable at $\beta \neq 0$, we focus on the ED results. Figure 4 (a)–(c) summarizes our findings for $\Delta = 1.5$ and $\beta J = 0.5$, 1, 2. We observe two effects. First, as the temperature is lowered, the number of momenta with diffusive density dynamics decreases. At $\beta J = 0.5$ and 1 the mode with $q = 0.11\pi$ still decays diffusively but for $\beta J = 2$ only the $q = 0$ mode displays diffusion. Second, as the temperature is lowered, D_q and τ_q increase significantly. For $q = 0$ this increase can be followed up to $\beta J = 2$. Fig. 4 (d) displays D_0 versus β in a semi-logarithmic plot for $\Delta = 1.5$ and 2.0. From this plot, one might be tempted to speculate on an exponential increase of D_0 with β beyond the temperature window depicted, see a related claim in Ref. 32. However, in view of the hydrodynamic relation $D_0 = t_0\, C_{J,0}(0)/C_{S,0}(0)$ this is a subtle issue. From our numerical analysis, we find $C_{S,0}(0)$ to be the dominant source of D_0's T-dependence for $0 < \beta J < 2$. But $C_{S,0}(0)$ is not $\propto \exp(c\beta)$ for all β [33]. An exponential increase of D_0 must further break down as $\beta \to \infty$ due to the finite spin gap for $\Delta > 1$. We also mention that, for $\Delta = 1$ and $\beta J \gg 1$, the dominant T-dependence of D_0 stems from $t_0 \propto 1/(T \ln T)$ [21, 22], which is not exponential.

Finally, we turn to a more detailed discussion of the temperature dependence of the critical momentum q_D. To this end, we first collect all momenta $q \lesssim q_D$ in Fig. 5. Then, to rationalize this, we invoke the standard hydrodynamics criterion that the relaxation time $1/(\tilde{q}^2 D_q)$ of a diffusive density mode should be larger than the decay time τ_q of the current, or equivalently, that a diffusive density spectrum should be narrower than the current spectrum, see Fig. 3. Therefore, breakdown of diffusion occurs at $\tilde{q}^2 D_q\, \tau_q \sim 1$, where we may set $D_q = D_0$ and $\tau_q = \tau_0$, due to the weak q-dependence of these quantities in our case. Based on our ED results for D_0 and τ_0, Fig. 5 displays the lines $\tilde{q}^2 D_0\, \tau_0 = 1$ versus β for both $\Delta = 1.5$ and 2.0 (solid curves). The obvious agreement between these lines and the boundaries for the collected values of $q \lesssim q_D$ is a convincing consistency check of our approach. Apparently, as β increases, q_D decreases. In view of the temperature dependence of D_0 and τ_0, this decrease is also approximately exponential for $0 \leq \beta J \lesssim 2$. To asses the relevance of finite size effects, Fig. 5 contains a comparison between the lines $\tilde{q}^2 D_0 \tau_0 = 1$ and the observed diffusive modes for $N = 16$ and 18 (symbols). Given the limited resolution of the q-grid, the agreement with these two system sizes is remarkably good.

In summary we have investigated magnetization transport in the spin-1/2 XXZ chain above the isotropic point at finite temperature and momentum. We found an extended momentum-space region of spin-diffusion with an approximately time and momentum independent diffusion constant. The diffusion cut-off wave vector (diffusion constant) was found to scale approximately linear with the (inverse) anisotropy and to decrease (increase) strongly with the inverse temperature.

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* r.steinigeweg@tu-bs.de

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